FASTMATH

Block Structured AMR Libraries and Their Interoperability with Other Math Libraries

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Some slides provided by Ann Almgren and Brian Van Straalen

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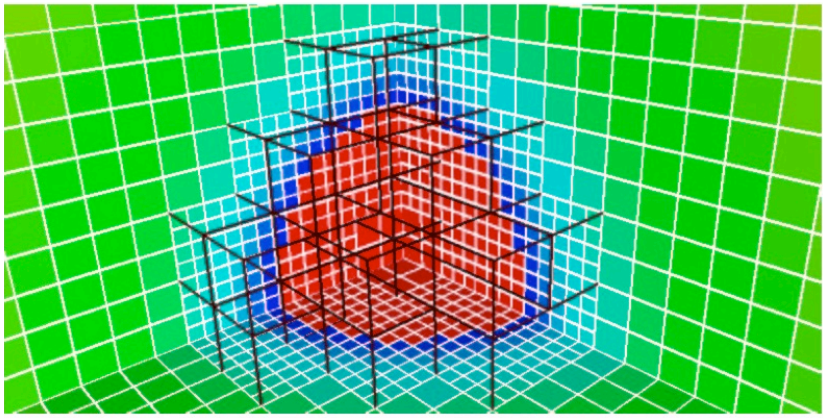
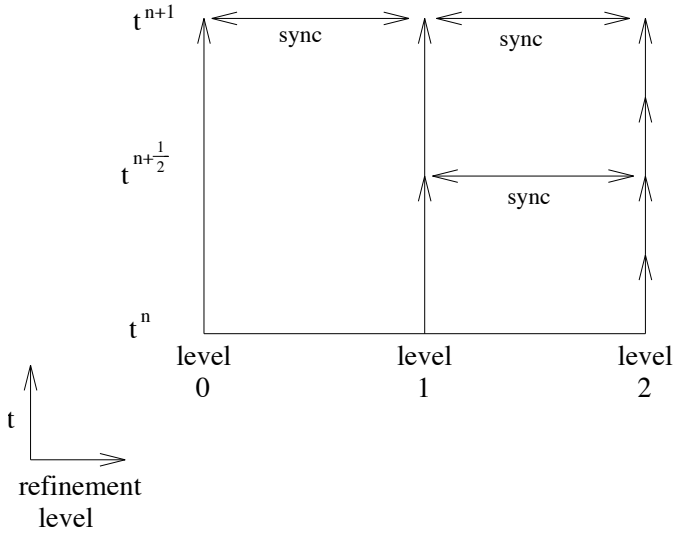
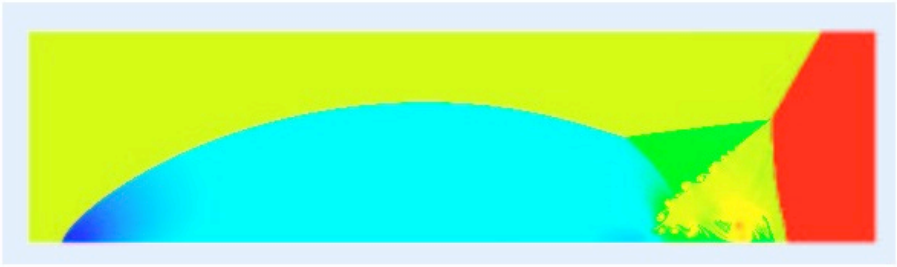
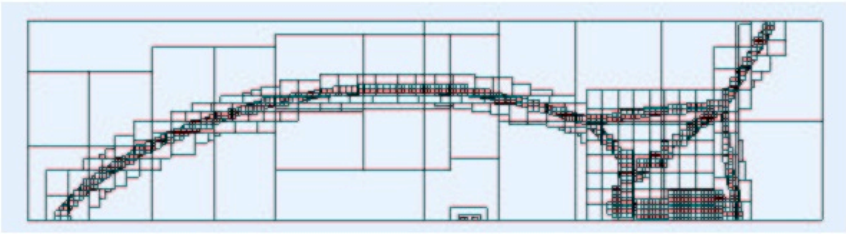
Block-Structured Local Refinement (Berger and Oliger, 1984)





Refined regions are organized into logically-rectangular patches.
Refinement is performed in time as well as in space.





FASTMATH

Why use AMR and When ?

- Think of AMR as a compression technique for the discretized mesh
- Apply higher resolution in the domain only where it is needed
- When should you use AMR:
  - When you have a multi-scale problem
  - When a uniformly spaced grid is going to use more memory than you have available to achieve the resolution you need
- You cannot always use AMR even when the above conditions are met
- When should you not use AMR:
  - When the overhead costs start to exceed gains from compression
  - When fine-coarse boundaries compromise the solution accuracy beyond acceptability

Much as using any tool in scientific computing, you should know what are the benefits and limits of the technologies you are planning to use

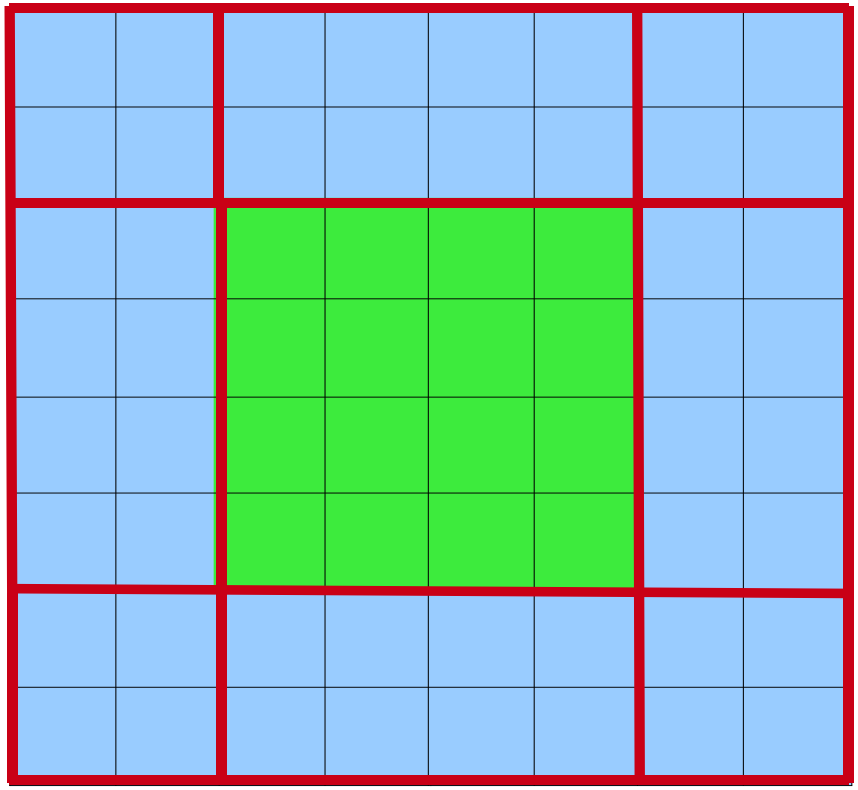
The Flip Side - Complexity

- Machinery needed for computations :
  - Interpolation, coarsening, flux corrections and other needed resolutions at fine-coarse boundaries

- Machinery needed for house keeping :
  - The relationships between entities at the same resolution levels
  - The relationships between entities at different resolution levels

- Machinery needed for parallelization :
  - Domain decomposition and distribution among processors
    - Sometimes conflicting goals of maintaining proximity and load balance
  - Redistribution of computational entities when the grid changes due to refinement
  - Gets more complicated when the solution method moves away from explicit solves

Abstraction for Explicit Methods

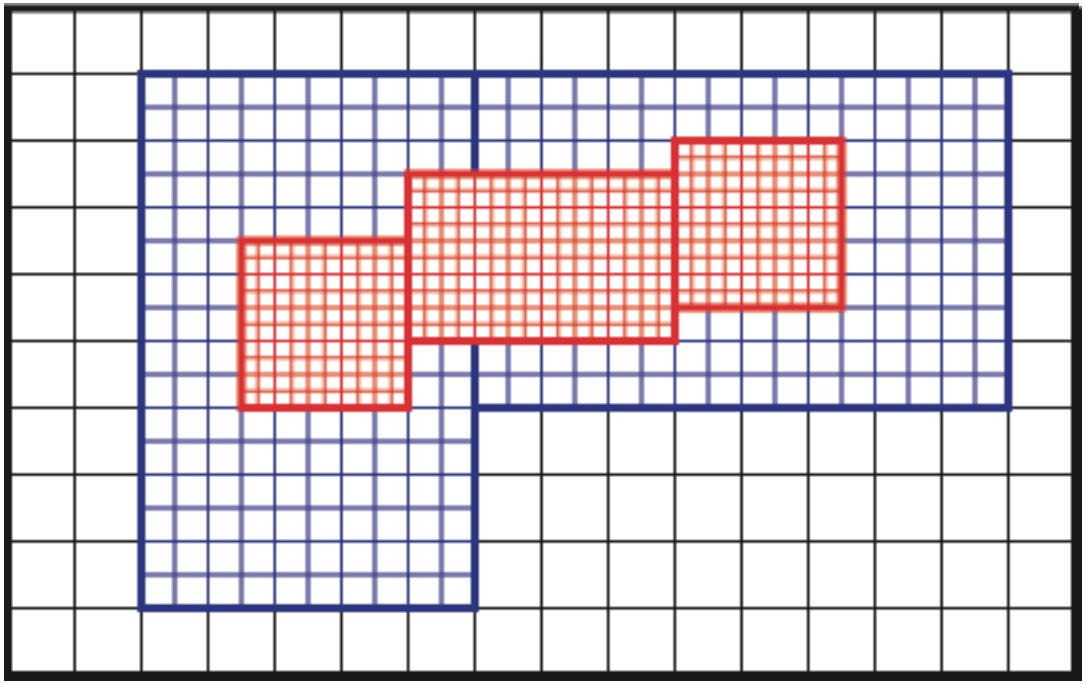


- A self contained computational domain
- Apply computational stencils
- The halo cells may come from same level exchanges or from a coarser level through interpolation
- If there is no sub-cycling, the interface is simple, all patches can get their halos filled simultaneously
- With sub-cycling either the application or the infrastructure can control what to fill when

Most structured AMR methods use the same abstraction for semi-implicit solvers such as multigrid, in the sense they operate on a block/box at a time, the operations in between and the orchestration gets more complicated

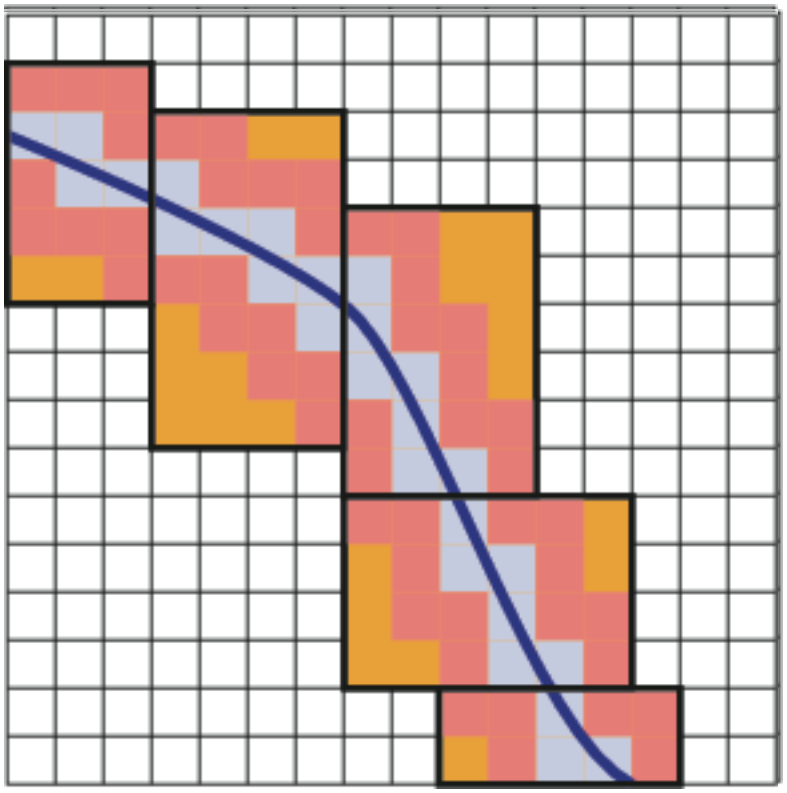
Approach

- Locally refine patches where needed to improve the solution.
- Each patch is a logically rectangular structured grid.
  - Better efficiency of data access.
  - Can amortize overhead of irregular operations over large number of regular operations.
- Refined grids are dynamically created and destroyed.

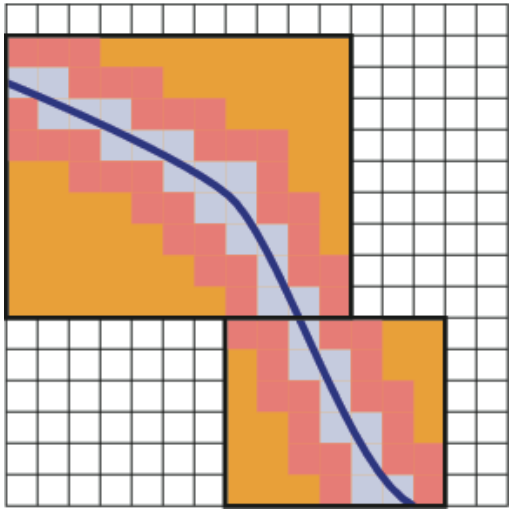


Building the Initial Hierarchy

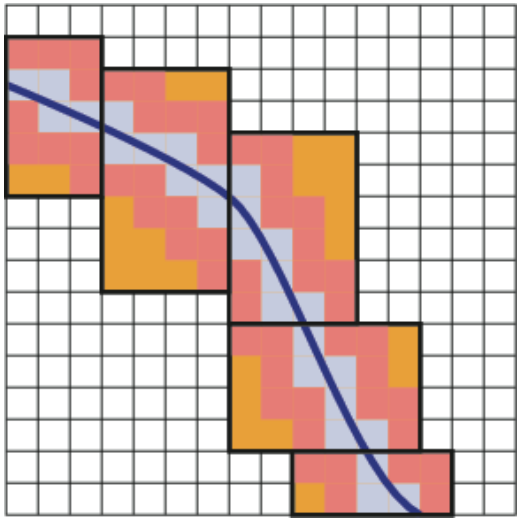
- Fill data at level 0
- Estimate where refinement is needed
- Group cells into patches according to constraints (refinement levels, grid efficiency etc)
- Repeat for the next level
- Maintain proper nesting



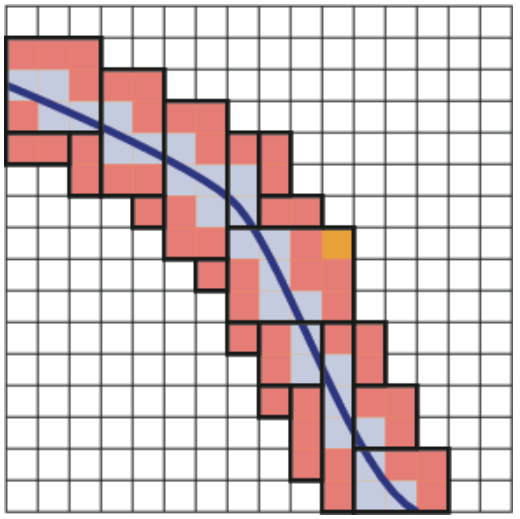
How Efficiency Affects the Grid



Efficiency=0.5



Efficiency=0.7



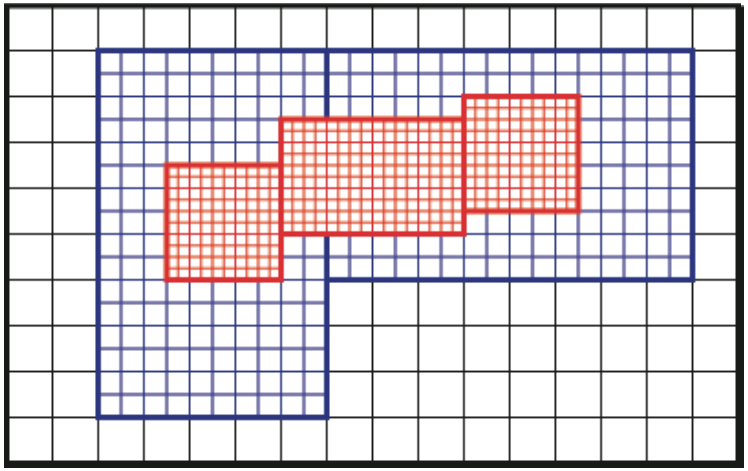
Efficiency=0.9

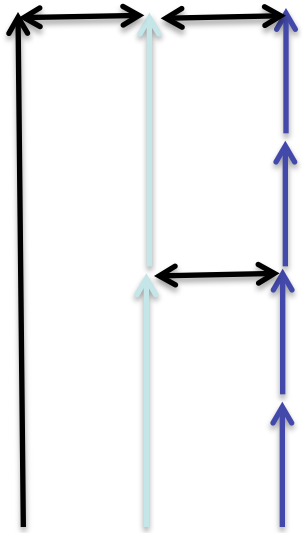
Adaptive in Time

- Consider two levels, coarse and fine with refinement ratio r

$$\Delta x_f = \Delta x_c / r \quad , \quad \Delta t_f = \Delta t_c / r,$$

- Advance
- Advance f $t_c \rightarrow t_c + \Delta t_c$
- Synchronize fine and coarse data
- Apply recursively to all refinement levels



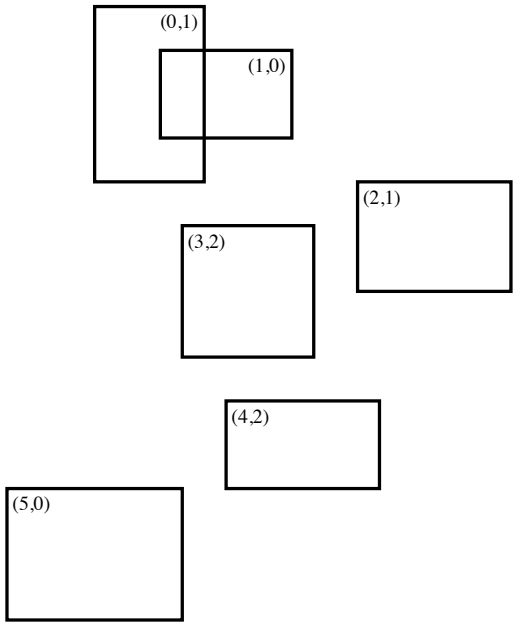


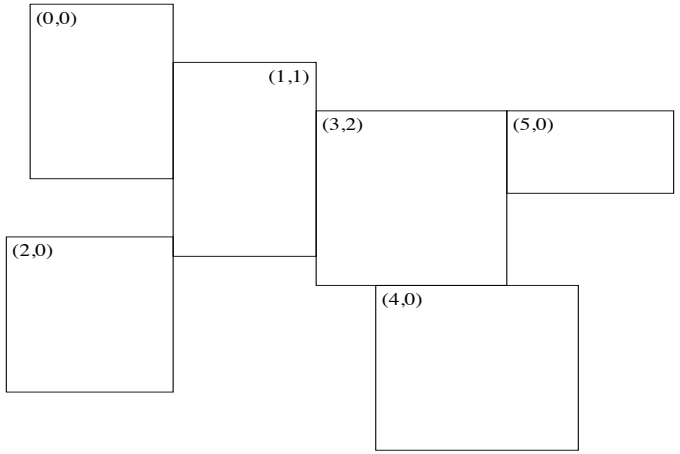
The Two Packages: Boxlib and Chombo

- Mixed-language model: C++ for higher-level data structures, Fortran for regular single-grid calculations.
- Reuseable components. Component design based on mapping of mathematical abstractions to classes.
- Build on public-domain standards: MPI.Chombo also uses HDF5
- Interoperability with other tools: VisIt, PETSc,hypre.
- The lowest levels are very similar – they had the same origin
- Examples from Chombo

Distributed Data on Unions of Rectangles

Provides a general mechanism for distributing data defined on unions of rectangles onto processors, and expressing communications between processors.

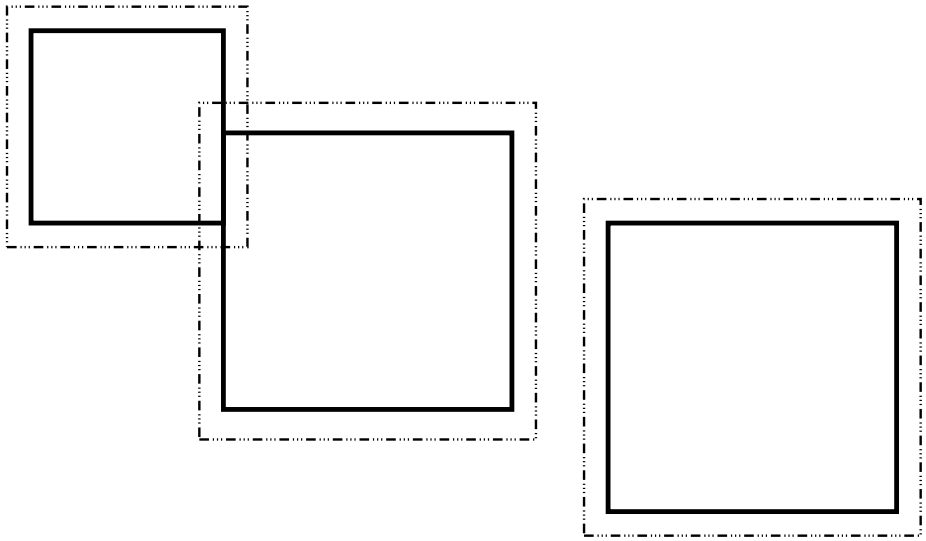




Metadata, of which all processors have a copy. `BoxLayout` is a collection of `Boxes` and processor assignments: $\{B_k,p_k\}_{k=1,ngrids}$. `DisjointBoxLayout:public Boxlayout` is a `BoxLayout` for which the `Boxes` must be disjoint

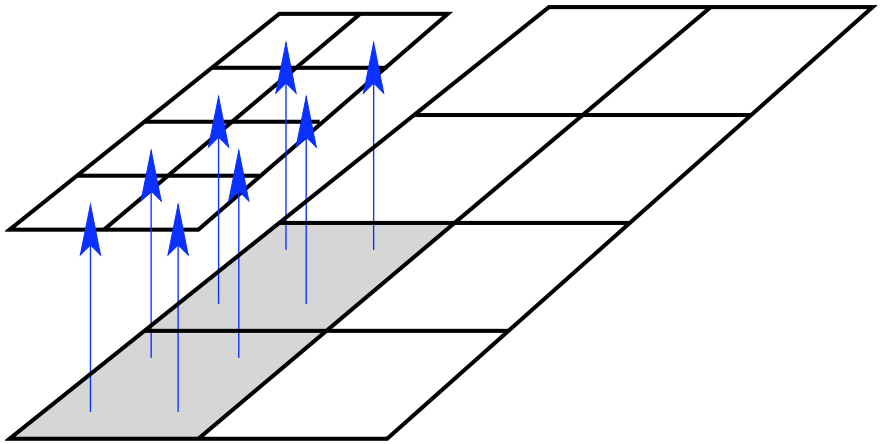
Data on Unions of boxes

Distributed data associated with a `DisjointBoxLayout`. Can have ghost cells around each box to handle intra-level, inter-level, and domain boundary conditions. Templated (LevelData) in Chombo.



Interpolation from coarse to fine

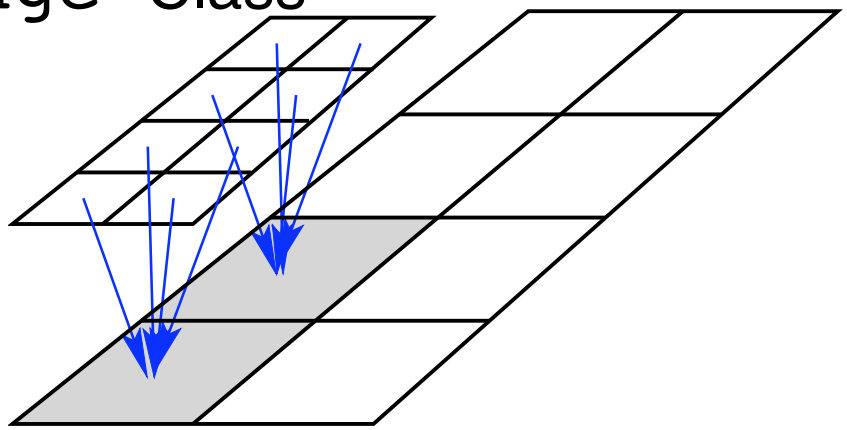
- Linearly interpolates data from coarse cells to the overlaying fine cells.
- Useful when initializing newly-refined regions after regridding.



Example:

```
ProblemDomain fineDomain;
DisjointBoxLayout coarseGrids, fineGrids;
int refinementRatio, nComp;
LevelData<FArrayBox> coarseData(coarseGrids, nComp);
LevelData<FArrayBox> fineData(fineGrids, nComp);

FineInterp interpolator(fineGrids, nComp, refinementRatio,
                        fineDomain);

// fineData is filled with linearly interpolated coarseData
interpolator.interpToFine(fineData, coarseData);
```

CoarseAverage Class



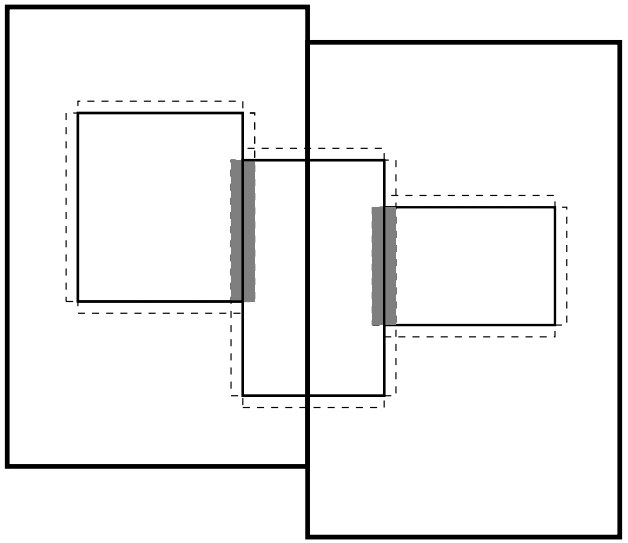
- Averages data from finer levels to covered regions in the next coarser level.
- Used for bringing coarse levels into sync with refined grids covering them.

Example:

```
DisjointBoxLayout fineGrids;
DisjointBoxLayout crseGrids;
int nComp, refRatio;

LevelData<FArrayBox> fineData(fineGrids, nComp);
LevelData<FArrayBox> crseData(crseGrids, nComp);

CoarseAverage averager(fineGrids, crseGrids, nComp,
refRatio);

averager.averageToCoarse(crseData, fineData);
```

Coarse-Fine Interactions (`AMRTools`)

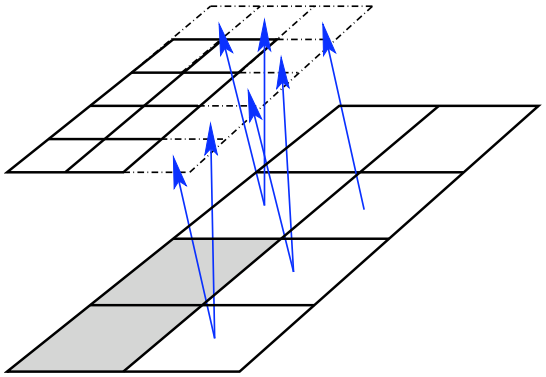
The operations that couple different levels of refinement are among the most difficult to implement, as they typically involve a combination of interprocessor communication and irregular computation.



- Interpolation between levels (`FineInterp`).
- Averaging down to coarser grids (`CoarseAverage`).
- Interpolation of boundary conditions (`PiecewiseLinearFillpatch`, `QuadCFInterp`, higher-order extensions).
- Managing conservation at refinement boundaries (`LevelFluxRegister`).

PiecewiseLinearFillPatch Class

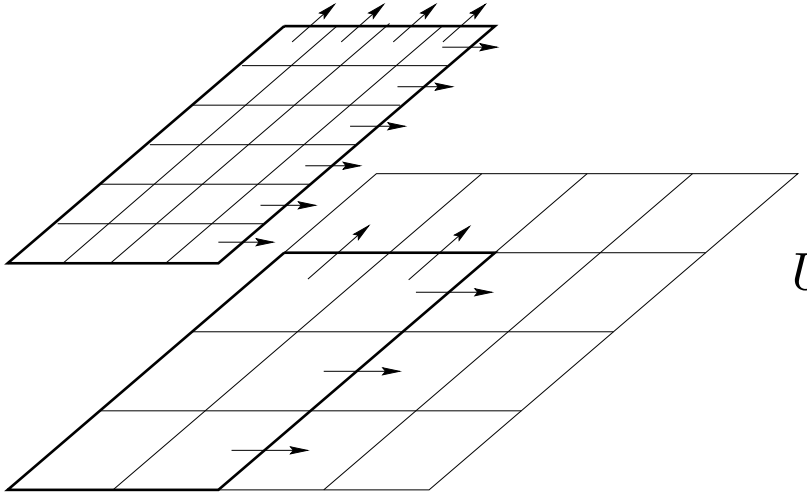
Linear interpolation of coarse-level data (in time and space) into fine-level ghost cells.



Example:

```
ProblemDomain crseDomain;
DisjointBoxLayout crseGrids, fineGrids;
int nComp, refRatio, nGhost;
Real oldCrseTime, newCrseTime, fineTime;

LevelData<FArrayBox> fineData(fineGrids, nComp,
nGhost*IntVect::Unit);
LevelData<FArrayBox> oldCrseData(crseGrids, nComp);
LevelData<FArrayBox> newCrseData(crseGrids, nComp);

PiecewiseLinearFillPatch filler(fineGrids, coarseGrids, nComp,
                                crseDomain, refRatio, nGhost);
Real alpha = (fineTime-oldCrseTime)/(newCrseTime-oldCrseTime);
filler.fillInterp(fineData, oldCrseData, newCrseData, alpha,
                  0, 0, nComp);
```

LevelFluxRegister Class



$$U^c := U^c + \Delta t^c (F^{c,s}_{\boldsymbol{i}^c - \frac{1}{2}\boldsymbol{e}} - \frac{1}{Z} \sum_{\boldsymbol{i}^f} F^{f,s}_{\boldsymbol{i}^f - \frac{1}{2}\boldsymbol{e}})$$

The coarse and fine fluxes are computed at different points in the program, and on different processors. We rewrite the process in the following steps.

$$\delta F = 0$$

$$\delta F := \delta F - F^c$$

$$\delta F := \delta F + < F^f >$$

$$U^c := U^c + D_R(\delta F)$$

Example: explicit heat equation solver on a single grid.

```
c Fortran code:
      subroutine heatsub2d(phi,nlphi0, nhphi0,nlphi1, nhphi1,
     &     nlreg, nhreg, dt, dx, nu)

      real*8  phi(nlphi0:nhphi0,nlphi1:nhphi1)
      real*8 dt,dx,nu
      integer nlreg(2),nhreg(2)

c Remaining declarations, setting of boundary conditions goes here.

       do j = nlreg(2), nhreg(2)
         do i = nlreg(1), nhreg(1)
            lapphi = (phi(i+1,j) +phi(i,j+1) +phi(i-1,j) +phi(i,j-1)
     &                -4.0d0*phi(i,j))/(dx*dx)

            phi(i,j) = phi(i,j) + nu*dt*lapphi
         enddo
       enddo

      return
      end
```

Example: explicit heat equation solver on a single grid.

```
// C++ code:

  Box domain(IntVect:Zero,(nx-1)*IntVect:Unit);
  FArrayBox soln(grow(domain,1), 1);
  soln.setVal(1.0);

  for (int nstep = 0;nstep < 100; nstep++)
 {
  heatsub2d_(soln.dataPtr(0),
           &(soln.loVect()[0]), &(soln.hiVect()[0]),
           &(soln.loVect()[1]), &(soln.hiVect()[1]),
             domain.loVect(), domain.hiVect(),
             &dt, &dx, &nu)
 }
```

ChomboFortran

ChomboFortran is a set of macros used by Chombo for:

- Managing the C++ / Fortran Interface.
- Writing dimension-independent Fortran code.

Advantages to ChomboFortran:

- Enables fast (2D) prototyping, and nearly immediate extension to 3D.
- Simplifies code maintenance and duplication by reducing the replication of dimension-specific code.

Previous C++/Fortran Interface

- C++ call site:

```
heatsub2d_(soln.dataPtr(0),
           &(soln.loVect()[0]), &(soln.hiVect()[0]),
           &(soln.loVect()[1]), &(soln.hiVect()[1]),
             domain.loVect(), domain.hiVect(),
             &dt, &dx, &nu);
```

- Fortran code:

```
                subroutine heatsub2d(phi,iphilo0, iphihi0,iphilo1,
iphihi1,
     &                        domboxlo, domboxhi, dt, dx, nu)

      real*8  phi(iphilo0:iphihi0,iphilo1:iphihi1)
      real*8 dt,dx,nu
      integer domboxlo(2),domboxhi(2)
```

Managing such an interface is error-prone and dimensionally dependent (since 3D will have more index arguments for array sizing).

C++ / Fortran Interface with ChomboFortran

- C++ call site:

```
FORT_HEATSUB(CHF_FRA(soln),
             CHF_BOX(domain),
             CHF_REAL(dt), CHF_REAL(dx), CHF_REAL(nu));
```

- Fortran code:

```
subroutine heatsub(CHF_FRA[phi], CHF_BOX[domain],
  &                CHF_REAL[dt], CHF_REAL[dx], CHF_REAL[nu])
```

ChomboFortran expands the argument lists on both sides depending on the dimensionality of the problem. On the Fortran side, it also generates the type declarations for the arguments automatically, along with appropriate header files to be included in the C++ code.

Dimension-independence with ChomboFortran

- Looping macros: `CHF_MULTIDO`
- Array indexing: `CHF_IX`

Replace

```
          do j = nlreg(2), nhreg(2)
         do i = nlreg(1), nhreg(1)
            phi(i,j) = phi(i,j) + nu*dt*lphi(i,j)
         enddo
      enddo
```

with

```
CHF_MULTIDO[dombox; i;j;k]
        phi(CHF_IX[i;j;k]) = phi(CHF_IX[i;j;k])
    &                      + nu*dt*lphi(CHF_IX[i;j;k])
     CHF_ENDDO
```

Prior to compilation, ChomboFortran replaces the indexing and looping macros with code appropriate to the dimensionality of the problem.

Elliptic Solver Example: `LinearSolver` virtual base class

```
class LinearSolver<T>

{

// define solver

virtual void define(LinearOp<T>* a_operator, bool
a_homogeneous) = 0;


// Solve L(phi) = rhs

virtual void solve(T& a_phi, const T& a_rhs) = 0;

...

}
```

`LinearOp<T>` defines what it means to evaluate the operator (for example, a Poisson Operator) and other functions associated with that operator. `T` can be an `FArrayBox` (single grid), `LevelData<FArrayBox>` (single-level), `Vector<LevelData<FArrayBox>*>` (AMR hierarchy).

Matrix representation of operators

- We have seen how construct AMR operator in Chombo as series of sub-operations
  - Coarse interpolation, fine interpolation, boundary conditions, etc.
- Matrix-free operators
  - Low memory: good for performance and memory complexity
  - Can use same technology to construct matrix-free equation solvers
    - Operator inverse
    - Use geometric multigrid (GMG)
    - Inherently somewhat isotropic
- Some applications have complex geometry and/or anisotropy
  - GMG looses efficacy
  - Solution: algebraic multigrid (AMG)
- Need explicit matrix representation of operator
  - Somewhat complex bookkeeping task but pretty mechanical
  - Recently developed infrastructure in Chombo support matrix construction
  - Apply series of transformations to matrix or stencil
    - Similar to operator but operating matrix/stencil instead of field data
  - Stencil: list of <Real weight, <cell, level>>
    - Stencil + map <cell, level> to global equation number: row of matrix
  - Start with A^0 : initial operator matrix
    - Eg, 1D 3-point stencil: {<-1.0, <i-1,lev>, <2.0, <i,lev>, <-1.0, <i+1,lev>}

PETSc Composite Grid Solvers: `PetscCompGrid`

```
class LinearSolver<T>

{

virtual void createOpStencil(IntVect,int,const
DataIndex&,StencilTensor &) = 0;

PetscErrorCode createMatrix(int a_makePmat=0);

Mat getMatrix() const { return m_mat;

}

class PetscCompGridPois : public PetscCompGrid

{

void createOpStencil(IntVect,int,const
DataIndex&,StencilTensor &);

}
```

PETSc Composite Grid Example: `PetscCompGridPois`

```
void

PetscCompGridPois::createOpStencil( IntVect a_iv, int a_ilev,const
DataIndex &a_di_dummy, StencilTensor &a_sten)

{
  Real dx=m_dxs[a_ilev][0],idx2=1./(dx*dx);
  StencilTensorValue &v0 = a_sten[IndexML(a_iv,a_ilev)];
  v0.define(1);
  v0.setValue(0,0,m_alpha - m_beta*2.*SpaceDim*idx2);
  for (int dir=0; dir<CH_SPACEDIM; ++dir) {
   for (SideIterator sit; sit.ok(); ++sit) {
     int isign = sign(sit());
     IntVect jiv(a_iv); jiv.shift(dir,isign);
     StencilTensorValue &v1 = a_sten[IndexML(jiv,a_ilev)];
     v1.define(1);
     v1.setValue(0,0,m_beta*idx2);
}}}
```

PETSc AMR Solver Example: releasedExamples/AMRPoisson/execPETSc

```
Solve(Vector<DisjointBoxLayout> grids, Vector<LevelData<FArrayBox> *> phi, Vector<LevelData<FArrayBox> *> rhs)
{
 PetscCompGridPois petscop(0.,-1.,s_order);
 RefCountedPtr<ConstDiriBC> bcfunc =
                         RefCountedPtr<ConstDiriBC>(new
                         ConstDiriBC(1,petscop.getGhostVect()));
 BCHolder bc(bcfunc);
 petscop.define( cdomains, grids, refratios, bc, cdx*RealVect::Unit );
 ierr = petscop.createMatrix(); CHKERRQ(ierr);
 Mat A = petscop.getMatrix();
 ierr = MatGetVecs(A,&x,&b); CHKERRQ(ierr);
 ierr = petscop.putChomboInPetsc(rhs,b); CHKERRQ(ierr);
 ierr = KSPCreate(PETSC_COMM_WORLD, &ksp); CHKERRQ(ierr);
 ierr = KSPSetOperators(ksp, A, A); CHKERRQ(ierr);
 ierr = KSPSetFromOptions(ksp); CHKERRQ(ierr);
 ierr = KSPSolve(ksp, b, x); CHKERRQ(ierr);
 ierr = KSPDestroy(&ksp); CHKERRQ(ierr);
 ierr = a_petscop.putPetscInChombo(x, phi); CHKERRQ(ierr);
}
```

Approach as matrix transformations

- We can think of these transformations as matrix or operators operating on one global matrix (not a good way to implement)
  - Range and domain space of these operators is critical

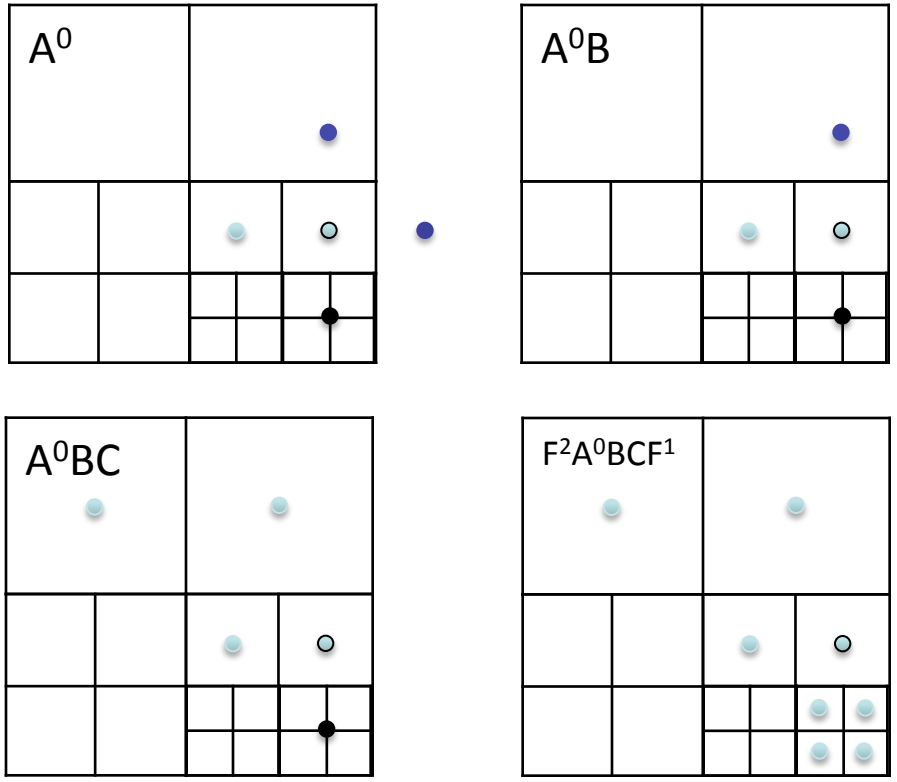
- Start with A^0 : initial operator matrix

- B: Boundary conditions for ghost cells off of domain
  - Need one op. for each direction (for corner points)
- C: Interpolate ghost cells on domain (supported by coarse cells)
- F: interpolate cells covered with fine cells
  - F removes covered cells from range and domain:
    Needs two operators F^2 & F^1
    left and right application

    Result: $A := F^2 \bullet A^0 \bullet B \bullet C \bullet F^1$

Approach from Stencil view

- Start with raw op stencil A^0, 5-point stencil
- 4 types of cells:
  - Valid (*V*)
    - Real degree of freedom cell in matrix
  - Boundary (*B*)
    - Ghost cell off of domain - BC
  - Coarse (*C*)
    - Ghost cell in domain
  - Fine (*F*)
    - Coarse cell covered by fine
- "raw" operator stencil A^0 composed of all 4 types
  - Transform stencil to have only valid cells
- B, C & F operator have
  - *domain space* with all types (ie, *B*, *C*, *F*)
  - range space w/o its corresponding cell type
    - That is, each operator filters its type
  - Thus after applying B, C & F only valid cells remain
  - Note, F removes *F* cells from range and domain:
    - Needs two operators F^2 & F^1
    - left and right application



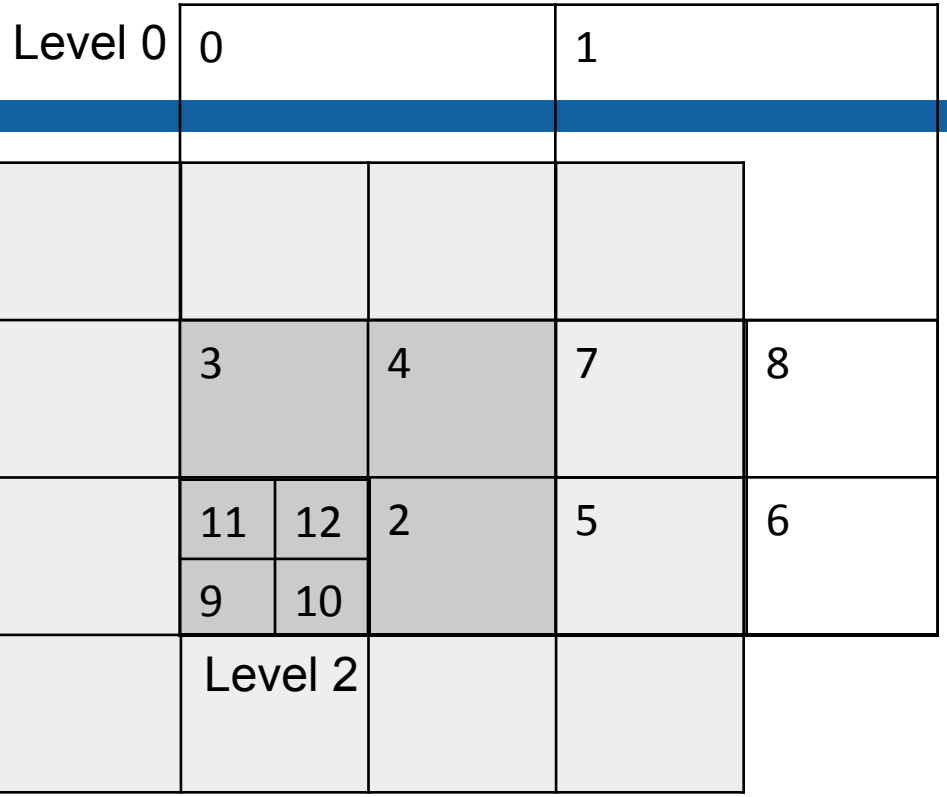
Cartoon of stencil for cell ○ as it is transformed

Example: Laplacian with 3 AMR levels

(dx = $6^{1/2}$ on level 1)

(**Invalid testing region!!!**)

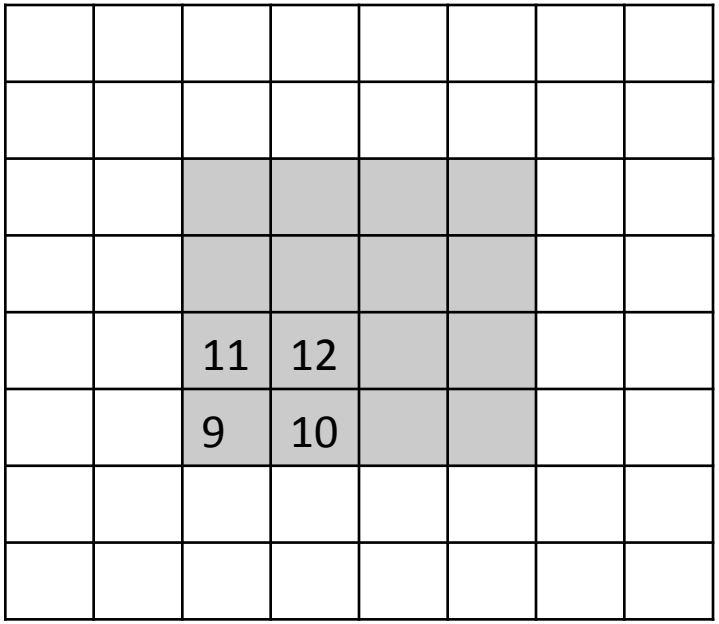
Problem domain – global cell IDs

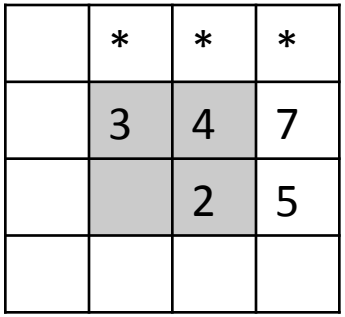


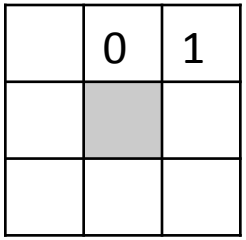
Extended patch <level=1, patch=0>

local cell IDs (implicit ordering from box iterators)

12	13	14	15
8	9	10	11
4	5	6	7
0	1	2	3







level 2 to global IDs (GIDs) for <1,0> → Level 1 GIDs for <1,0> → Level 0 GIDs for <1,0>

Initial FABMatrix A^0

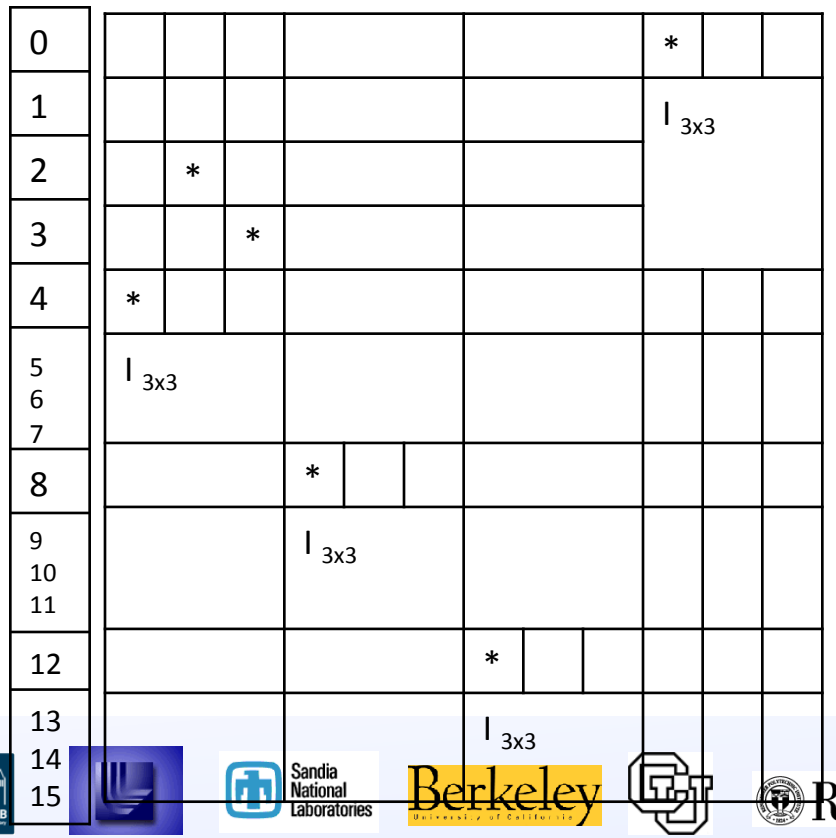
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
5	-1	-4	-1		-4	20	-4		-1	-4	-1					
6		-1	-4	-1		-4	20	-4		-1	-4	-1				
9					-1	-4	-1		-4	20	-4		-1	-4	-1	
10						-1	-4	-1		-4	20	-4		-1	-4	-1

Local IDs on level 1.
Simplify notation:
eg, 5 == <5,1>

FABMatrix B
* = -1 for Dirichlet
* = 1 for Neumann.
Use higher order in practice.
Split operator into SpaceDim parts (x & y here).

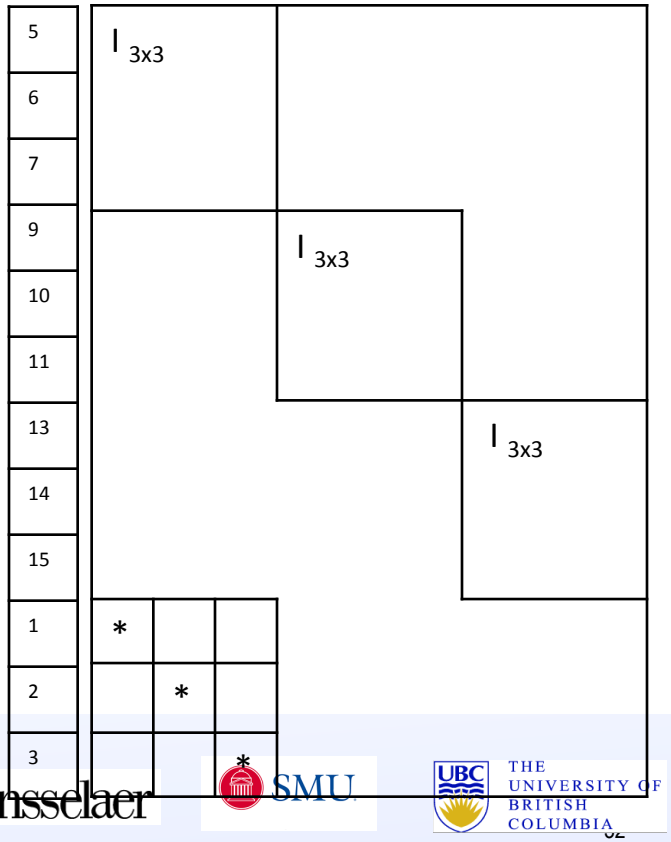
B^x

5	6	7	9	10	11	13	14	15	1	2	3



B^y

5	6	7	9	10	11	13	14	15



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Polytropic Gas Example

- Demonstrates integration of conservative laws (e.g., the Euler equations of gas dynamics) on an AMR grid hierarchy.
- Uses unsplit, second-order Godunov method.
- One of the released examples in Chombo distribution
- Look under $CHOBO_HOME/releasedExamples/AMRGodonov/execPolytropic
- Source code:
  - AMRLevel specialized for this set of problems in ../srcPolytropic
  - Main in ./amrGodunov.cpp
  - The executable name includes options used in the build
    amrGodunov2d.Linux.64.g++.gfortran.OPTHIGH.ex
    - Compiled using g++ and gfortran
    - High optimization
    - For Linux
    - No MPI
  - We use ramp.inputs to provide runtime parameters

Parameters

Length of the run
- godunov.max_step = 200
- godunov.max_time = 0.064

Shape of the patch
- # godunov.num_cells = 32 8 4
- godunov.num_cells = 64 16 8

Grid refinement parameters
- godunov.max_level = 2

For 2D
- godunov.ref_ratio = 4 4 4 4 4

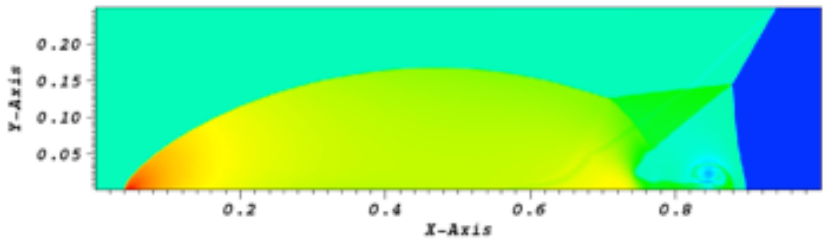
For 3D
- # godunov.ref_ratio = 2 2 2 2 2

Regridding parameters
- godunov.regrid_interval = 2 2 2 2 2 2
- godunov.tag_buffer_size = 3
- godunov.refine_thresh = 0.015

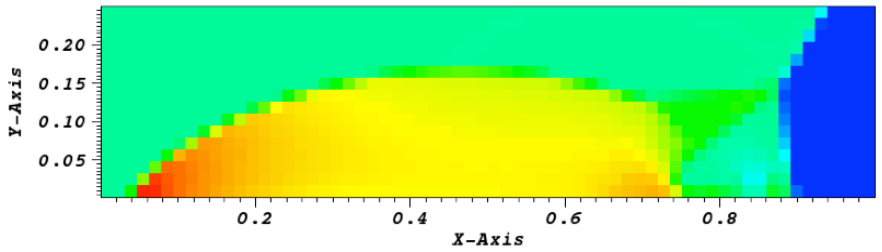
Grid generation parameters
- godunov.block_factor = 4
- godunov.max_grid_size = 32
- godunov.fill_ratio = 0.75

Experimenting with Parameters

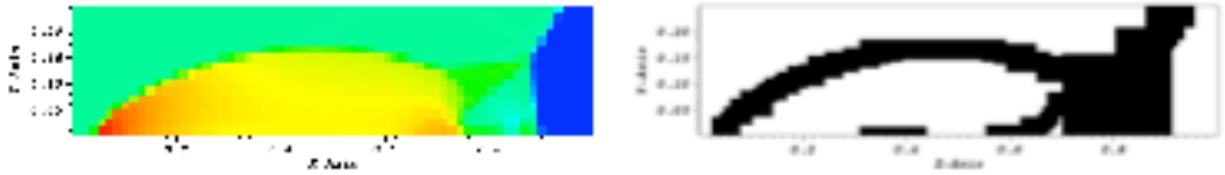
Default



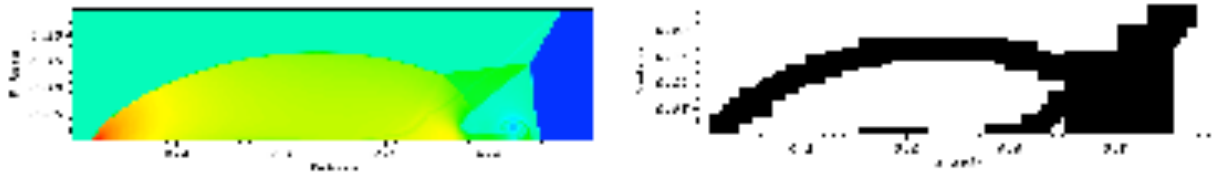
Change ref_ratio to 2



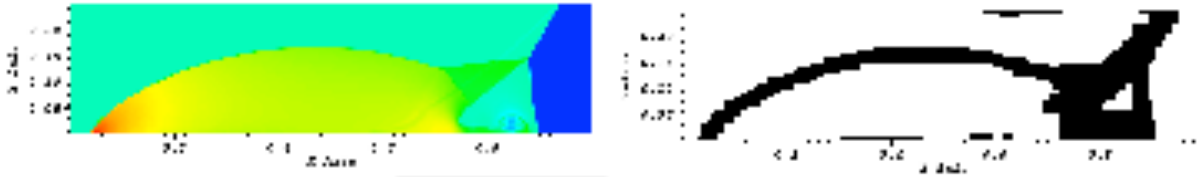
2 levels, refinement ratio of 2



2 levels, refinement ratio of 4



4 levels, refinement ratio of 2



Variations in output with change in refinement parameters

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